A First Course on Kinetics and Reaction Engineering
Unit 35. Zoned Reactor Models

Overview

Unit 35 considers zoned reactor models, also called compartment models. Sometimes a reactor that is expected to obey the assumptions of an ideal reactor fails to do so, and the failure can be attributed to a physical issue that causes the flow to be different from that in an ideal reactor. For example, the baffles in a CSTR might not be sized or positioned properly leading to “pockets” of fluid that are not perfectly mixed with the rest of the fluid in the reactor. This reactor might be modeled as a CSTR in combination with a well-mixed stagnant zone. As a second example, a packed bed reactor might not perform like an ideal PFR because the packing is not properly distributed, causing some fraction of the flow to bypass most of the packed bed. A zoned reactor model might be developed for this system where one zone represents the primary flow through the bed and a second zone represents the bypassing fraction of the flow. In effect, zoned reactor models are multiple reactor networks that are being used to model a single physical reactor.

Learning Objectives

Upon completion of this unit, you should be able to perform the following specific tasks and be able to recognize when they are needed and apply them correctly in the course of a more complex analysis:

- Generate zoned reactor models consisting of PFR zones, CSTR zones and well-mixed stagnant CSTR zones to represent real reactors that fail to meet assumptions of an ideal CSTR or ideal PFR model
- Perform reaction engineering tasks using zoned reactor models

Information

Sometimes a reactor that was intended to obey the assumptions of one of the ideal reactor types fails to do so. As a consequence, predictions about the performance of the reactor will not be correct if they are based upon the ideal reactor model. There are two ways to try and bring the predictions of the model and the actual reactor performance back together: modify the reactor or the way it is operated so that it does obey the ideal reactor model, or modify the reactor model so that it accurately predicts the performance of the reactor. If the reactor is already set up and operational, and if its performance is acceptable, then the preferred approach may be to modify the reactor model. That way the operation of the reactor does not need to be interrupted. It is also likely that modifying the model will be more cost effective than modifying the actual reactor.

There can be a number of reasons why a reactor fails to obey the assumptions of one of the ideal reactor types. One possible reason is that the flow deviates from the assumptions inherent in the ideal reactor models. In some such cases, the reactor in question can be conceptually divided into two or more interconnected zones. Each zone can have idealized flow that can be modeled in a straightforward manner, and the zones can be connected together in an appropriate manner. In effect, this type of model replaces the single ideal reactor model with a network of CSTRs and PFRs. The flow into the reactor is split appropriately in an attempt to reproduce the non-ideal flow in the non-ideal reactor.

Developing a zoned reactor model requires some insight into the reason why the reactor in question does not obey the ideal reactor assumptions. In some cases the engineer's intuition may provide an idea. For example, suppose the catalyst packing in a packed bed reactor had to be replaced. Before the replacement the reactor performance was accurately described by the ideal PFR model, but after the change, the ideal PFR model is no longer sufficiently accurate. This might lead the engineer to suspect that the new catalyst packing is not properly distributed in the reactor and as a consequence, a fraction of the flow is bypassing part of the packed bed. This might be modeled as a two zone reactor consisting of two PFRs in parallel, as indicated schematically in Figure 35.1. Most of the flow in the model would pass through a PFR zone that represents the packed bed, while an appropriate fraction of the flow would pass through the other PFR zone that represents the bypassing flow. The split of the flow between the two zones and the residence time in the PFR zone representing the bypassing flow could be used as adjustable parameters to fit the zoned reactor model to match the actual performance of the reactor.

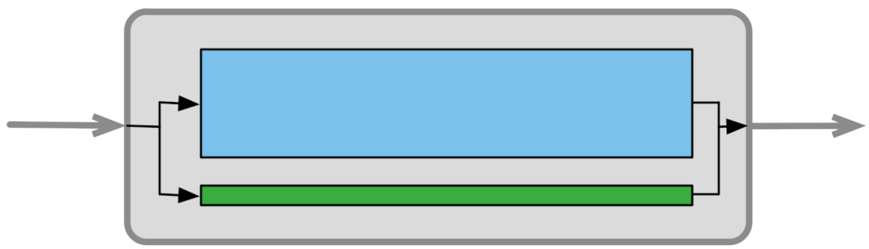
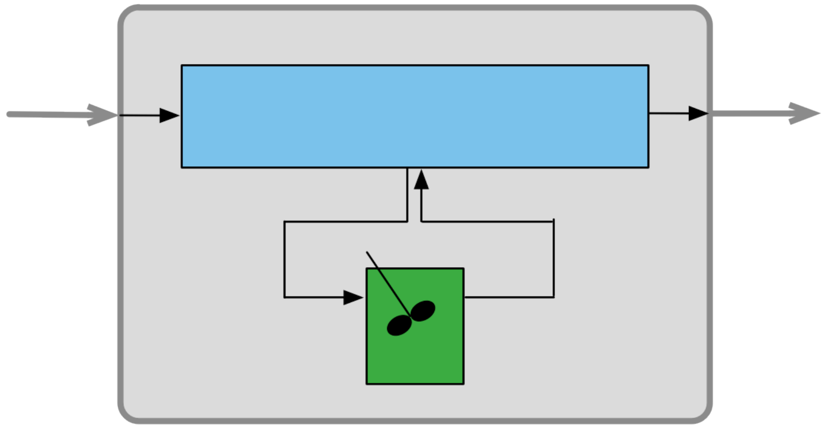


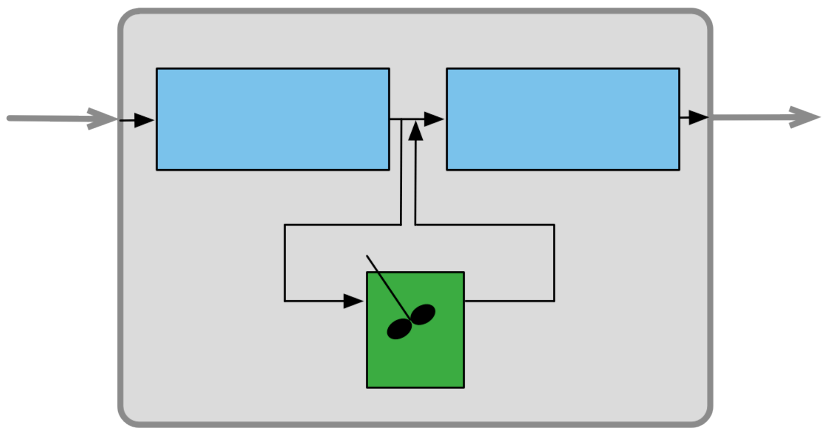
Figure 35.1. A schematic representation of a two-zone reactor model for a packed bed reactor (gray) with some fluid bypassing the majority of the bed. One of the two PFR zones represents the main packed bed reactor (blue) while the other represents the bypassing fluid (green).

The number of zones and ways of connecting them are innumerable, but three basic types of connection will cover the vast majority of situations. The first two types of zone connections are parallel and series. These are exactly the same as the reactor networks discussed in Unit 29. The third type of connection creates a "well mixed stagnant" zone by use of a CSTR zone. The difference is in the way a well mixed stagnant CSTR zone is connected to the other reactor zones. The inlet to the well mixed stagnant zone and the outlet from it both connect to another reactor zone at the same location. In effect, the well mixed stagnant CSTR zone draws some amount of fluid out of the reactor zone it is connected to while simultaneously replacing that withdrawn fluid with an equal amount taken from the well-mixed stagnant CSTR zone.

Figure 35.2 (a) shows a zoned reactor model where a well-mixed stagnant CSTR zone has been added to a PFR zone. Note, however, that the single PFR zone can be split into two PFR zones connected in series as long as the volume of the two zones equals that of the single zone. Splitting the PFR zone in this way does not change the performance (recall from Unit 29 that two PFRs in series are completely equivalent to a single PFR with a volume equal to the sum of the series PFRs). Thus, the zoned reactor model shown in Figure 35.2 (a) is completely equivalent to the alternative representation shown in Figure 35.2 (b).



(a)



(b)

Figure 35.2. Two completely equivalent ways of adding a well-mixed stagnant CSTR zone (green) to a PFR zone (blue) in a zoned reactor model (gray).

Figure 35.3 (a) shows a zoned reactor model where a well-mixed stagnant CSTR zone has been added to a regular CSTR zone. Note the inlet to the stagnant zone is drawn from the regular CSTR's contents and the outlet from the stagnant zone feeds back into the regular CSTR's contents. Noting that the contents of the regular CSTR zone are perfectly mixed, the feed into the stagnant zone could equally well be drawn from the outlet of the regular CSTR zone and the outlet from the stagnant zone could equally well be added to the feed to the regular CSTR zone. As a result, Figure 35.3 (b) is completely equivalent to Figure 35.3 (a).

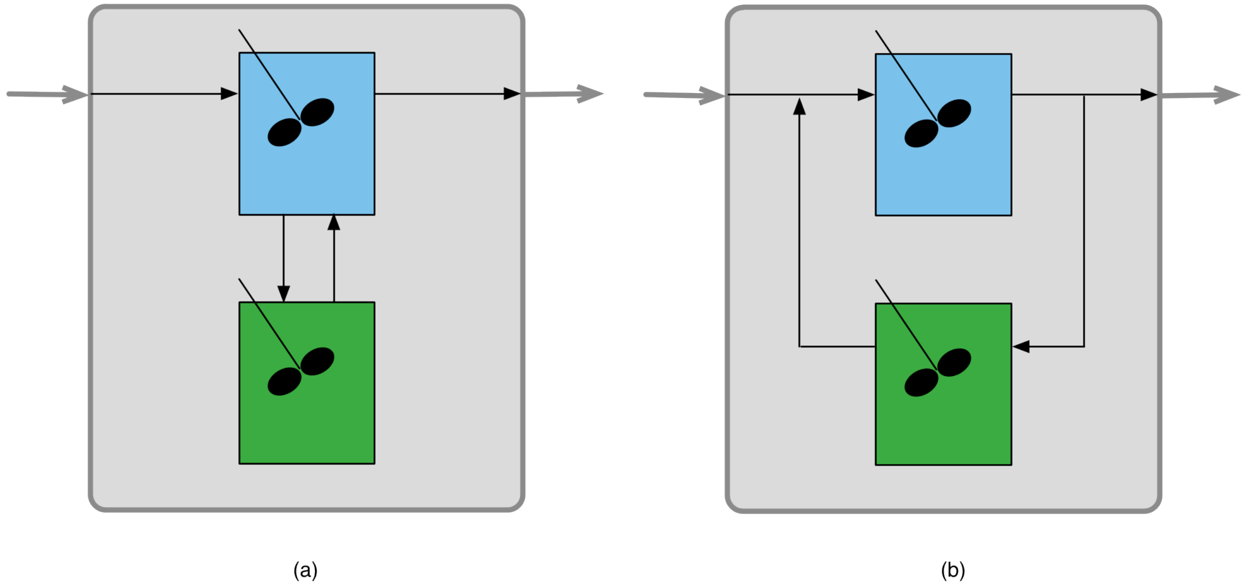


Figure 35.3. Two completely equivalent ways of adding a well-mixed stagnant CSTR zone (green) to a CSTR zone(blue) in a zoned reactor model (gray).

You may recall that Unit 29 showed that an infinite number of CSTRs connected in series shows performance that is identical to a PFR. Now suppose one had a tubular reactor that failed to fully obey the assumption of plug flow. That is, suppose a measurement of the age function for the reactor indicated that there was some small amount of axial mixing taking place. This reactor might be accurately modeled as a tubular reactor with axial dispersion, as discussed in Unit 33. An alternative approach would be to use a zoned reactor model where a large number of equally-sized CSTR zones are connected in series. We know from Unit 29, that as the number of zones approaches infinity, this zoned reactor model will approach an ideal PFR. As the number of zones decreases, the amount of axial mixing will decrease. Thus, the number of equally-sized CSTR zones can be used as an adjustable parameter in the zoned reactor model. That adjustable parameter can be chosen so that the resulting zoned reactor model most accurately predicts the performance of the actual, non-ideal tubular reactor.

The development of a zoned reactor model usually involves specifying values for one or more adjustable parameters. The adjustable parameters are typically relative sizes of the zones comprising the model and the fractional splits of flows between those zones. The best values for these adjustable parameters can be determined using a regression analysis like that described in Supplemental Unit S3 or S4. The data used for fitting can be actual reactor data (e. g. conversion and selectivity as a function of feed flow, composition and temperature) as well as age function data (see Unit 11). The solution of the design equations for a zoned reactor is exactly the same as the solution of the design equations for a reactor network as discussed in Unit 29.